



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 07:15 AM UTC

PDB ID : 9N5G / pdb_00009n5g
Title : RNA polymerase II elongation complex with 8-oxoG at +1 site, ATP in both A- and E-site
Authors : Oh, J.; Wang, D.
Deposited on : 2025-02-04
Resolution : 3.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

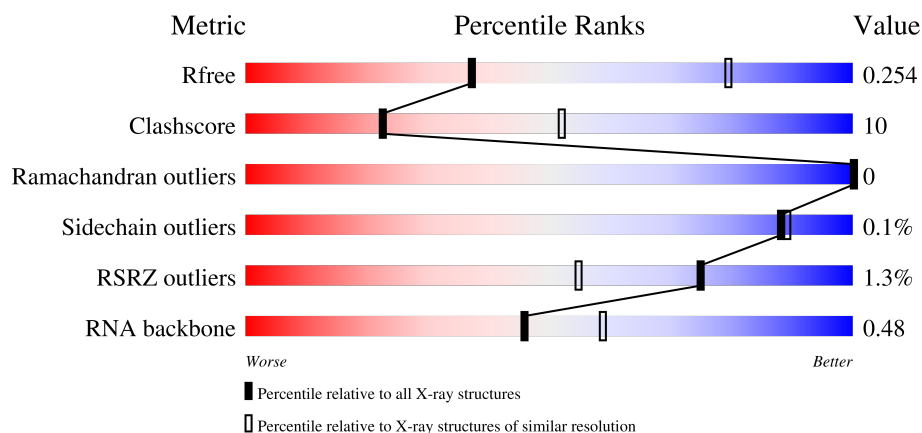
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)
RNA backbone	3983	1113 (3.42-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	9	44% 44% 11%
2	T	29	31% 52% 17%
3	N	18	17% 50% 33%
4	A	1733	61% 19% 20%

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Mol	Chain	Length	Quality of chain
5	B	1224	2% 70% 21% 8%
6	C	318	64% 20% 16%
7	E	215	67% 32% 1% 2%
8	F	155	42% 14% 45%
9	H	146	62% 29% 9%
10	I	122	75% 21% 2% 2%
11	J	70	66% 27% 7%
12	K	120	74% 21% 5%
13	L	70	49% 13% 39% 4%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 28998 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	9	Total	C	N	O	P	0	0	0
			199	88	40	62	9			

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	24	Total	C	N	O	P	0	1	0
			493	235	81	153	24			

- Molecule 3 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	12	Total	C	N	O	P	0	0	0
			256	119	58	67	12			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1385	Total	C	N	O	S	0	0	0
			10837	6836	1898	2043	60			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1121	Total	C	N	O	S	0	0	0
			8837	5595	1544	1645	53			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	213	Total	C	N	O	S	0	0	0
			1734	1102	304	317	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			684	437	115	129	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1052	664	173	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	118	Total	C	N	O	S	0	0	0
			946	582	170	184	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

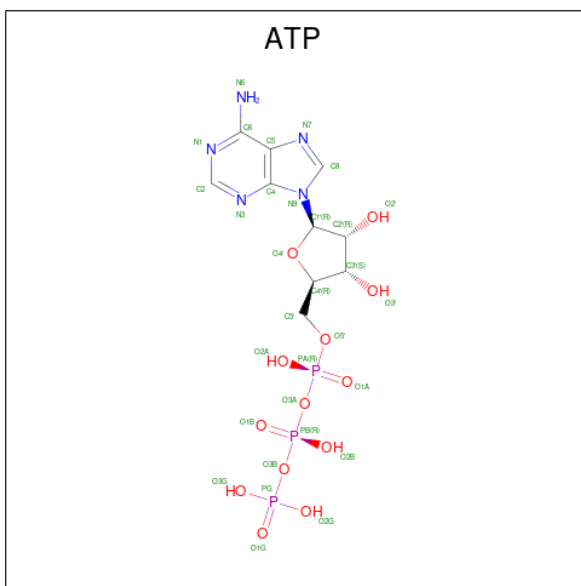
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	43	Total	C	N	O	S	0	0	0
			337	208	66	59	4			

- Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	R	1	Total	C	N	O	P	
			62	20	10	26	6	1

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	Zn	0	0
			2	2		
15	B	1	Total	Zn	0	0
			1	1		
15	C	1	Total	Zn	0	0
			1	1		
15	I	2	Total	Zn	0	0
			2	2		
15	J	1	Total	Zn	0	0
			1	1		
15	L	1	Total	Zn	0	0
			1	1		

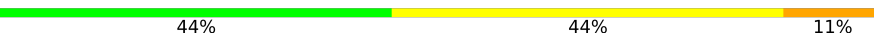
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

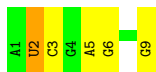
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

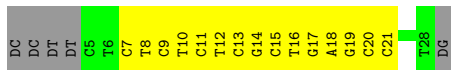
- Molecule 1: RNA

Chain R: 

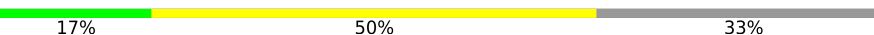


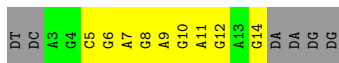
- Molecule 2: Template strand DNA

Chain T: 



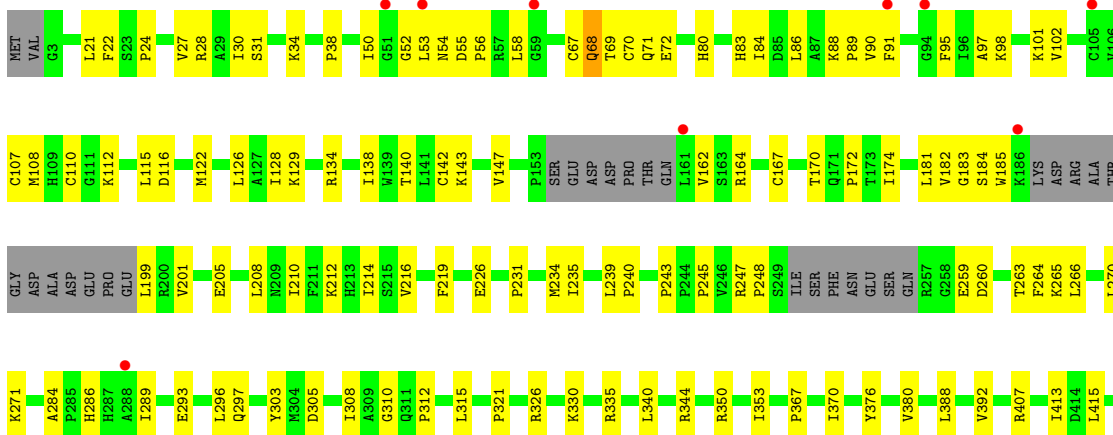
- Molecule 3: Non-template strand DNA

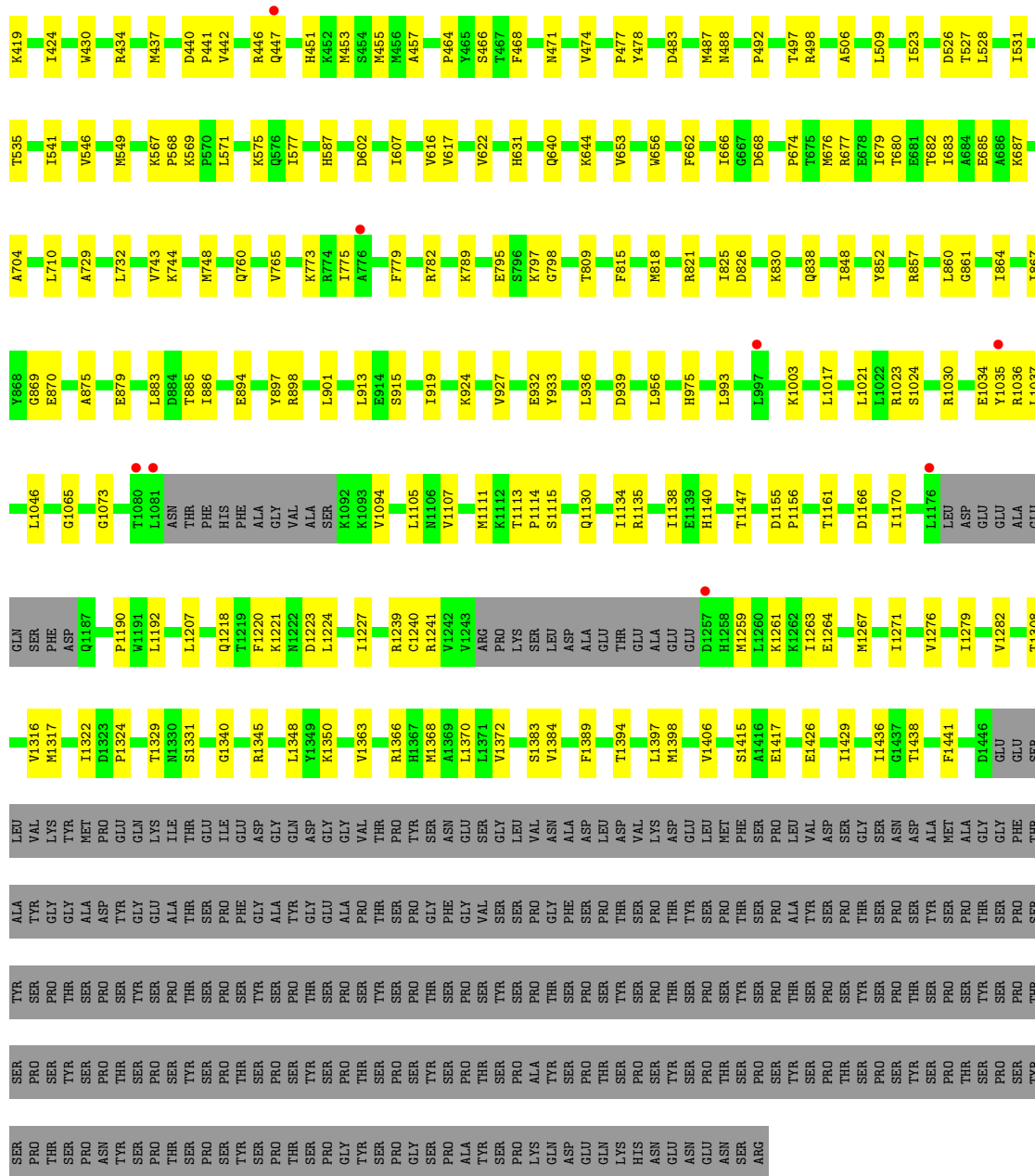
Chain N: 



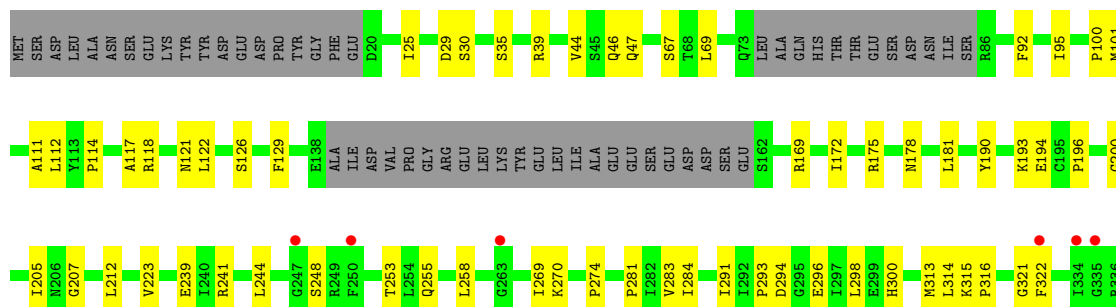
- Molecule 4: DNA-directed RNA polymerase II subunit RPB1

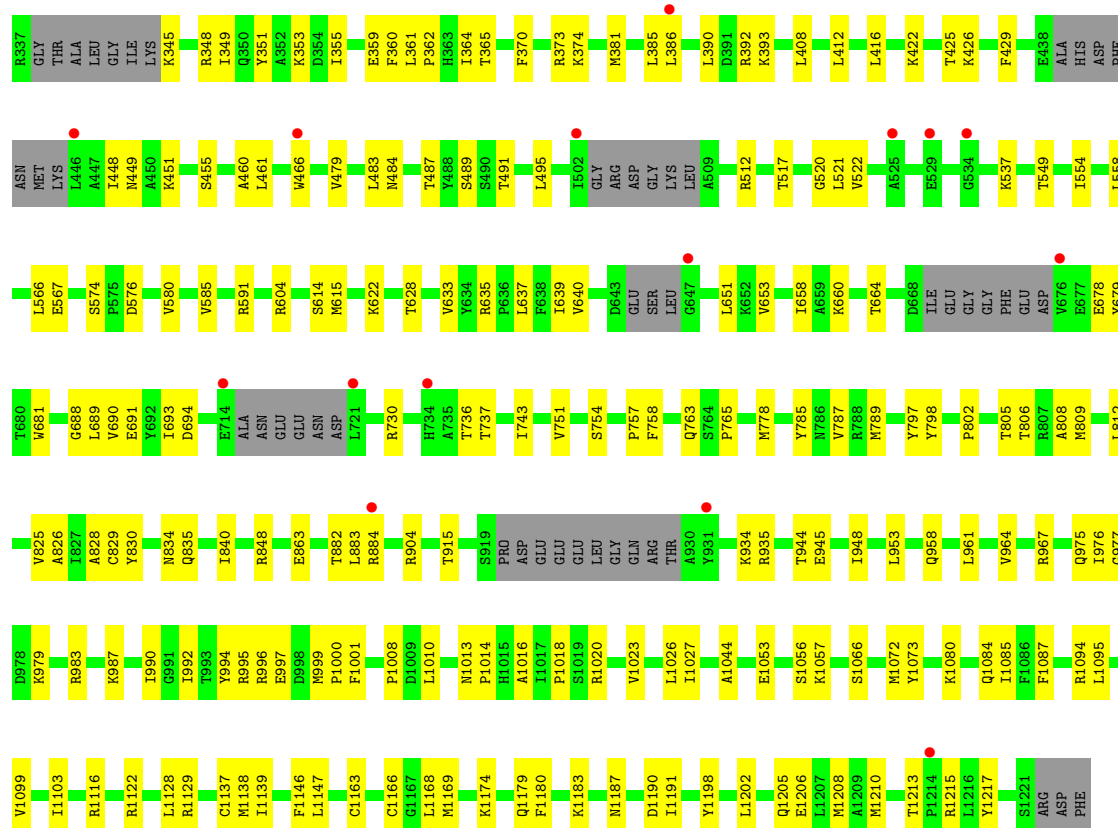
Chain A: 





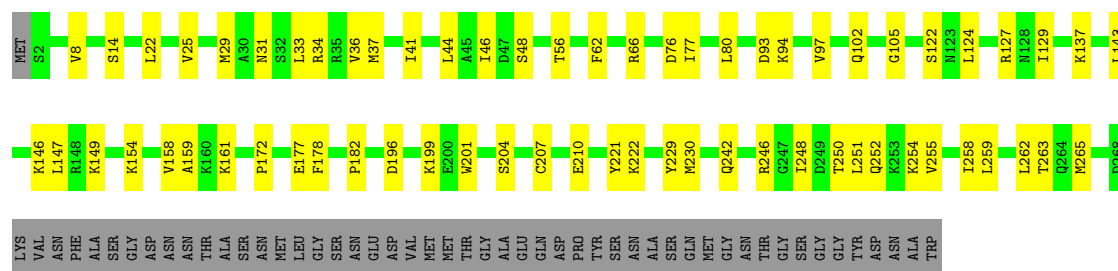
• Molecule 5: DNA-directed RNA polymerase II subunit RPB2





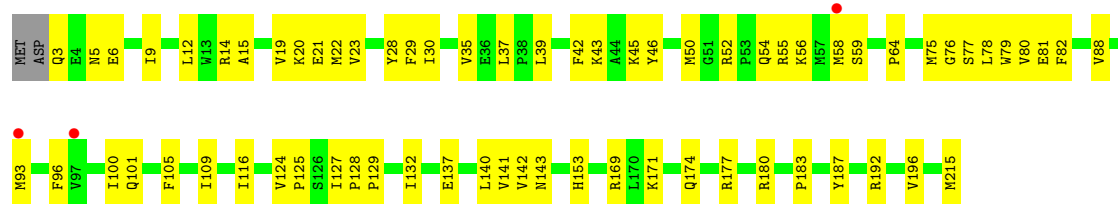
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

Chain C: 64% 20% 16%

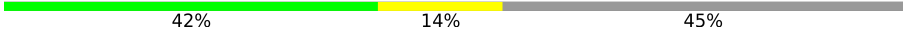


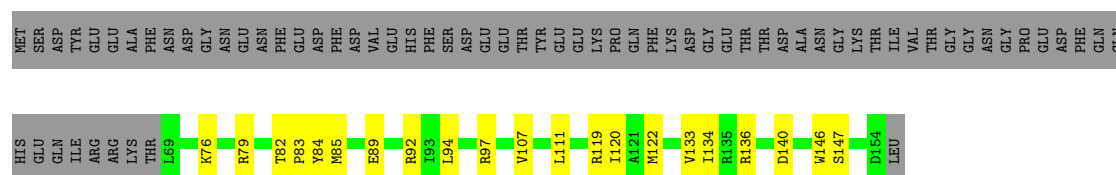
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 67% 32%



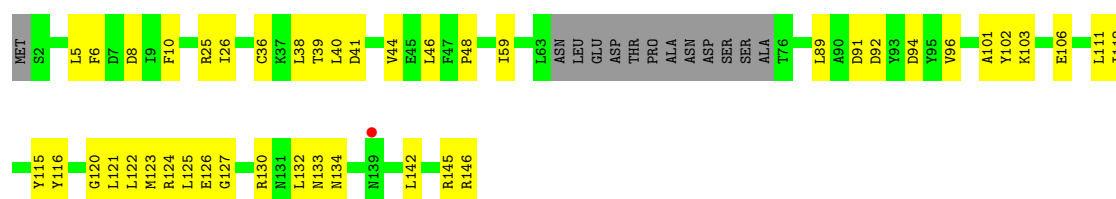
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 



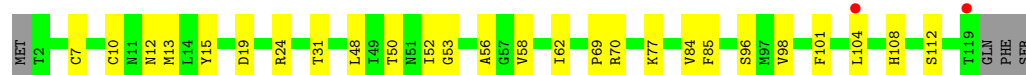
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 



- Molecule 10: DNA-directed RNA polymerase II subunit RPB9

Chain I: 



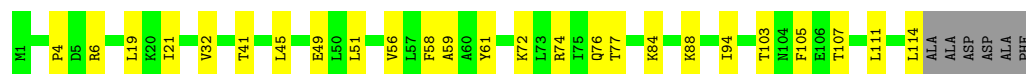
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 



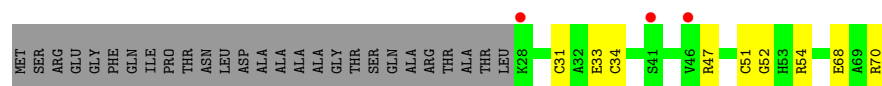
- Molecule 12: DNA-directed RNA polymerase II subunit RPB11

Chain K: 



- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.78Å 222.49Å 192.29Å 90.00° 98.10° 90.00°	Depositor
Resolution (Å)	48.06 – 3.15 48.06 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.06-3.15) 99.8 (48.06-3.15)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.220 , 0.254 0.221 , 0.254	Depositor DCC
R_{free} test set	2000 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å ²)	79.6	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 83.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28998	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 8OG, ZN, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	R	0.14	0/223	0.35	0/345
2	T	0.26	0/507	0.53	0/775
3	N	0.25	0/290	0.50	0/447
4	A	0.17	0/11029	0.37	1/14919 (0.0%)
5	B	0.15	0/9008	0.34	0/12158
6	C	0.17	0/2139	0.35	0/2899
7	E	0.14	0/1770	0.36	0/2383
8	F	0.14	0/696	0.33	0/943
9	H	0.15	0/1070	0.39	0/1452
10	I	0.14	0/964	0.34	0/1301
11	J	0.18	0/541	0.38	0/727
12	K	0.15	0/937	0.34	0/1265
13	L	0.16	0/339	0.37	0/450
All	All	0.16	0/29513	0.36	1/40064 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	68	GLN	CB-CA-C	-5.45	103.78	111.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	199	0	98	4	0
2	T	493	0	272	17	0
3	N	256	0	133	9	0
4	A	10837	0	10882	241	0
5	B	8837	0	8788	182	0
6	C	2101	0	2056	46	0
7	E	1734	0	1755	53	0
8	F	684	0	692	15	0
9	H	1052	0	1007	28	0
10	I	946	0	887	20	0
11	J	532	0	542	14	0
12	K	919	0	929	20	0
13	L	337	0	353	7	0
14	R	62	0	24	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	1	0	0	0	0
All	All	28998	0	28418	602	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 602 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:68:GLN:O	4:A:69:THR:HG22	1.59	1.02
4:A:284:ALA:HB1	4:A:289:ILE:HD11	1.50	0.93
7:E:46:TYR:HD2	7:E:58:MET:HG2	1.36	0.90
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.55	0.88
4:A:184:SER:HA	4:A:199:LEU:HD21	1.56	0.87

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1371/1733 (79%)	1331 (97%)	40 (3%)	0	100	100
5	B	1101/1224 (90%)	1076 (98%)	25 (2%)	0	100	100
6	C	265/318 (83%)	261 (98%)	4 (2%)	0	100	100
7	E	211/215 (98%)	204 (97%)	7 (3%)	0	100	100
8	F	84/155 (54%)	83 (99%)	1 (1%)	0	100	100
9	H	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
10	I	116/122 (95%)	116 (100%)	0	0	100	100
11	J	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
12	K	112/120 (93%)	110 (98%)	2 (2%)	0	100	100
13	L	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	3493/4173 (84%)	3407 (98%)	86 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1195/1520 (79%)	1194 (100%)	1 (0%)	88	89
5	B	953/1061 (90%)	953 (100%)	0	100	100
6	C	235/274 (86%)	235 (100%)	0	100	100
7	E	193/197 (98%)	193 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	F	73/137 (53%)	73 (100%)	0	100	100
9	H	114/128 (89%)	114 (100%)	0	100	100
10	I	109/116 (94%)	108 (99%)	1 (1%)	70	77
11	J	60/65 (92%)	60 (100%)	0	100	100
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	37/57 (65%)	37 (100%)	0	100	100
All	All	3068/3657 (84%)	3066 (100%)	2 (0%)	88	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	67	CYS
10	I	7	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
7	E	115	ASN
12	K	92	ASN
7	E	146	HIS
10	I	60	GLN
5	B	47	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/9 (88%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	9	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	8OG	T	19[B]	-	22,25,26	4.11	18 (81%)	26,37,40	1.78	7 (26%)
2	8OG	T	19[A]	-	22,25,26	4.11	18 (81%)	26,37,40	1.75	7 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8OG	T	19[B]	-	-	2/7/21/22	0/3/3/3
2	8OG	T	19[A]	-	-	2/7/21/22	0/3/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19[A]	8OG	C8-N7	7.32	1.51	1.38
2	T	19[B]	8OG	C8-N7	7.12	1.51	1.38
2	T	19[B]	8OG	C8-N9	6.53	1.52	1.40
2	T	19[A]	8OG	C8-N9	6.26	1.51	1.40
2	T	19[B]	8OG	C2-N3	6.19	1.48	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19[A]	8OG	C2-N3-C4	4.79	120.55	112.30
2	T	19[B]	8OG	C2-N3-C4	4.67	120.34	112.30
2	T	19[B]	8OG	N9-C4-N3	3.48	130.48	126.13
2	T	19[B]	8OG	C2-N1-C6	-3.19	119.33	125.11
2	T	19[A]	8OG	C2-N1-C6	-3.10	119.49	125.11

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19[A]	8OG	O4'-C4'-C5'-O5'
2	T	19[B]	8OG	O4'-C4'-C5'-O5'
2	T	19[A]	8OG	C3'-C4'-C5'-O5'
2	T	19[B]	8OG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	ATP	R	2101[B]	-	32,33,33	3.57	12 (37%)	48,52,52	2.39	12 (25%)
14	ATP	R	2101[A]	-	32,33,33	3.55	12 (37%)	48,52,52	2.29	12 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	ATP	R	2101[B]	-	-	5/22/38/38	0/3/3/3
14	ATP	R	2101[A]	-	-	6/22/38/38	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	R	2101[B]	ATP	C3'-C4'	-9.92	1.27	1.53
14	R	2101[A]	ATP	C3'-C4'	-9.81	1.28	1.53
14	R	2101[A]	ATP	C2'-C1'	-8.04	1.28	1.53
14	R	2101[B]	ATP	C2'-C1'	-8.00	1.28	1.53
14	R	2101[B]	ATP	O4'-C1'	6.29	1.56	1.42

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	R	2101[B]	ATP	N6-C6-N1	-8.69	99.01	118.38
14	R	2101[A]	ATP	N6-C6-N1	-7.86	100.86	118.38
14	R	2101[B]	ATP	C5-C6-N6	7.02	140.67	123.29
14	R	2101[A]	ATP	C5-C6-N6	6.28	138.84	123.29
14	R	2101[B]	ATP	N3-C2-N1	-5.60	120.10	128.58

There are no chirality outliers.

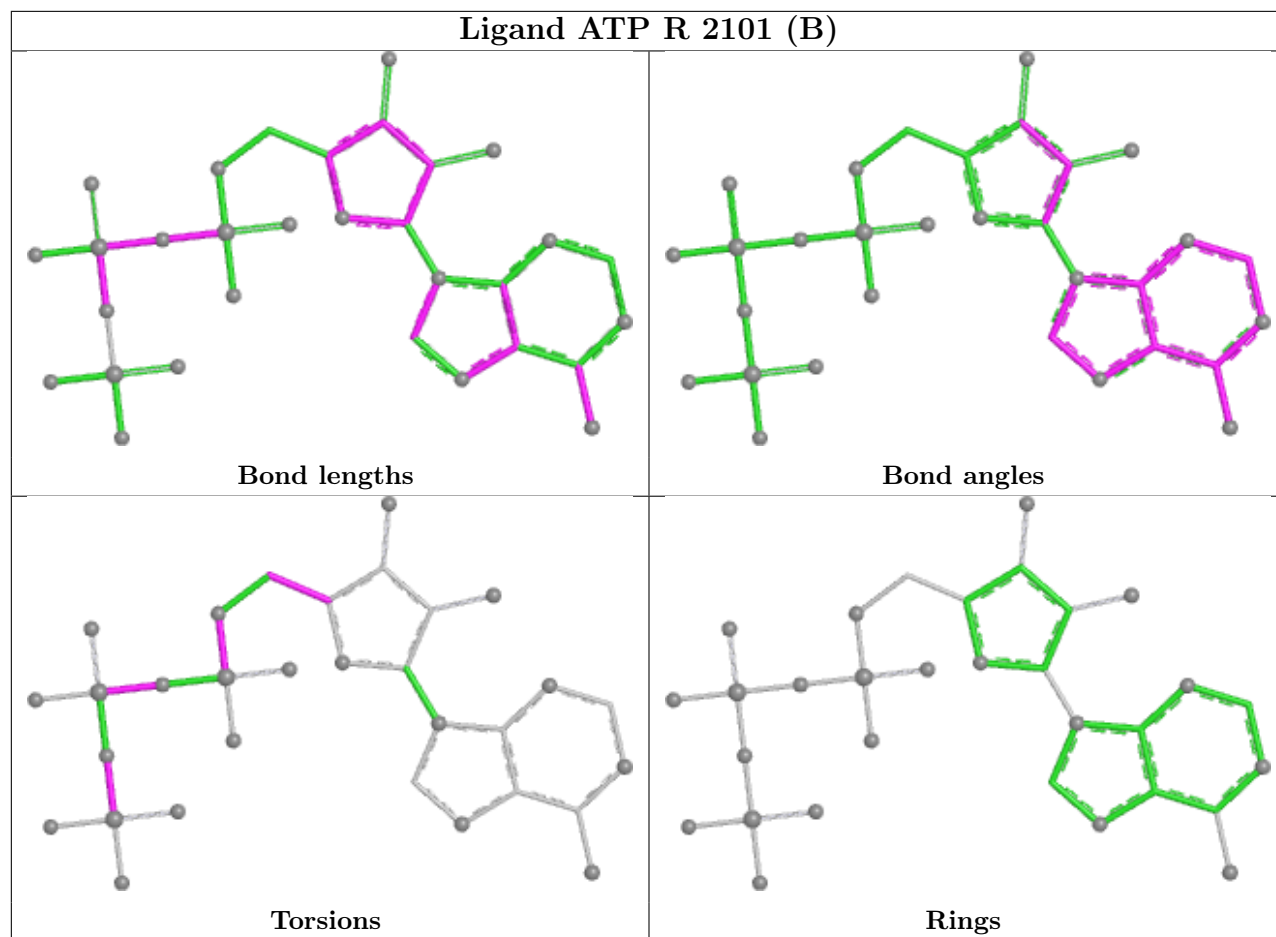
5 of 11 torsion outliers are listed below:

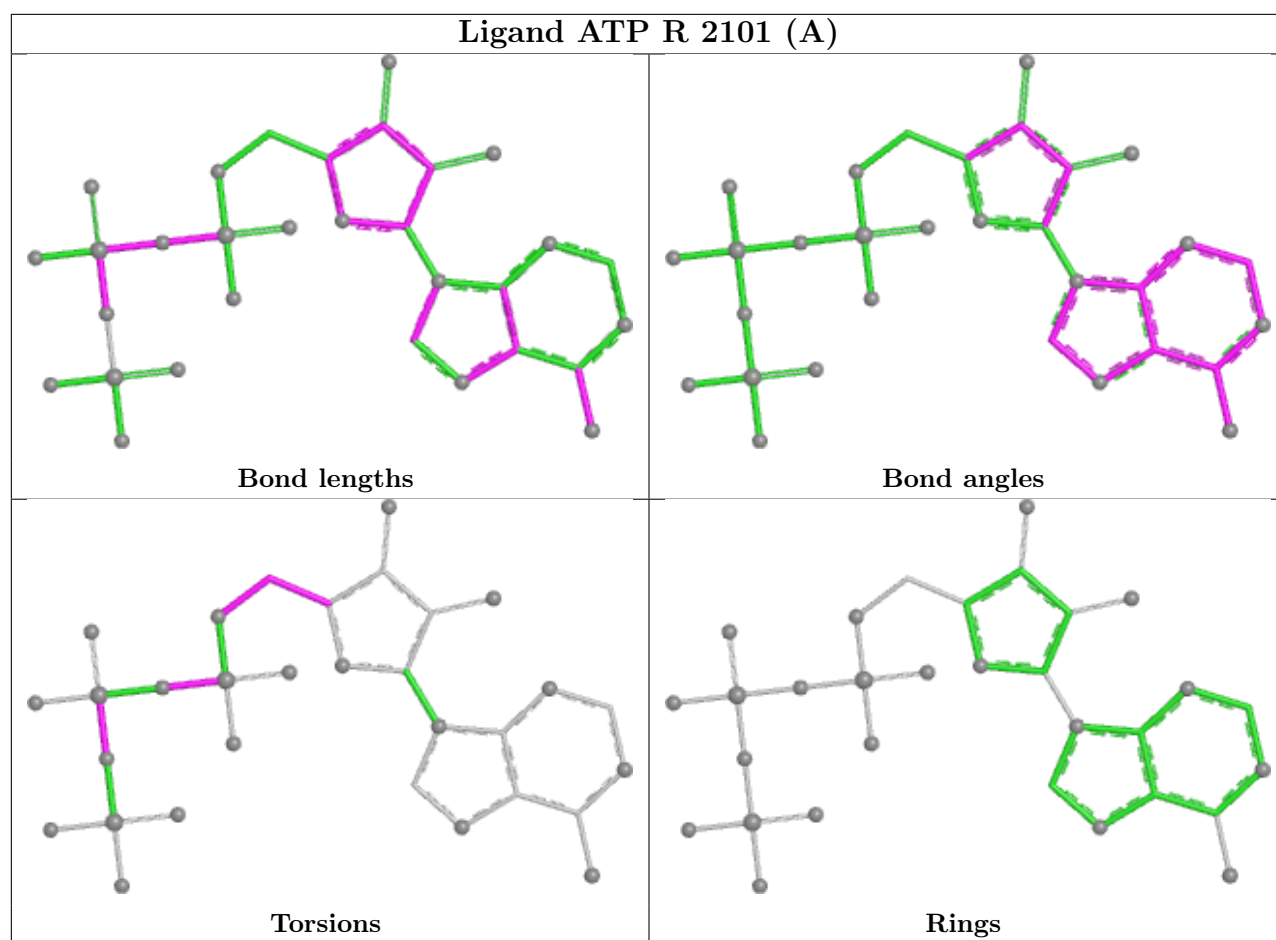
Mol	Chain	Res	Type	Atoms
14	R	2101[A]	ATP	PB-O3A-PA-O5'
14	R	2101[B]	ATP	PB-O3B-PG-O2G
14	R	2101[B]	ATP	C3'-C4'-C5'-O5'
14	R	2101[B]	ATP	O4'-C4'-C5'-O5'
14	R	2101[A]	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	9/9 (100%)	-0.00	0 100 100	93, 103, 199, 215	0
2	T	23/29 (79%)	0.17	0 100 100	88, 160, 258, 264	0
3	N	12/18 (66%)	0.21	0 100 100	151, 188, 267, 275	0
4	A	1385/1733 (79%)	0.00	17 (1%) 76 57	49, 91, 171, 274	0
5	B	1121/1224 (91%)	0.02	21 (1%) 66 45	43, 79, 147, 233	0
6	C	267/318 (83%)	-0.20	0 100 100	48, 79, 119, 166	0
7	E	213/215 (99%)	0.03	3 (1%) 73 53	68, 120, 184, 235	0
8	F	86/155 (55%)	-0.20	0 100 100	61, 96, 146, 212	0
9	H	133/146 (91%)	0.14	1 (0%) 82 66	79, 114, 173, 238	0
10	I	118/122 (96%)	0.05	2 (1%) 69 48	59, 102, 149, 200	0
11	J	65/70 (92%)	-0.07	1 (1%) 72 52	55, 71, 109, 142	0
12	K	114/120 (95%)	-0.27	0 100 100	51, 83, 121, 168	0
13	L	43/70 (61%)	0.79	3 (6%) 22 13	59, 151, 198, 273	0
All	All	3589/4229 (84%)	-0.00	48 (1%) 75 55	43, 89, 168, 275	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	714	GLU	5.6
4	A	1257	ASP	3.3
4	A	1081	LEU	3.2
7	E	93	MET	3.1
13	L	41	SER	3.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	8OG	T	19[A]	23/24	0.90	0.11	85,97,119,132	12
2	8OG	T	19[B]	23/24	0.90	0.11	85,97,119,132	12

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

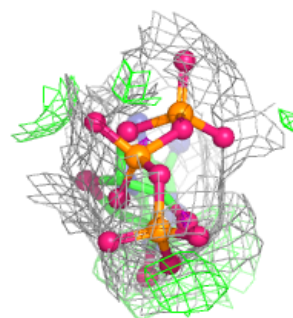
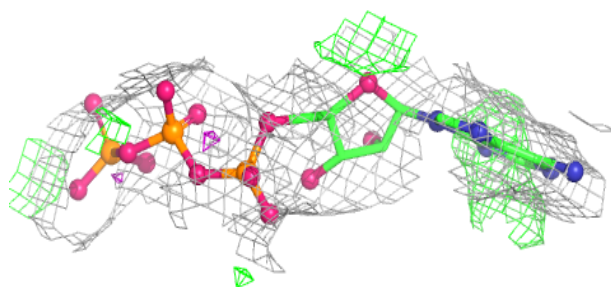
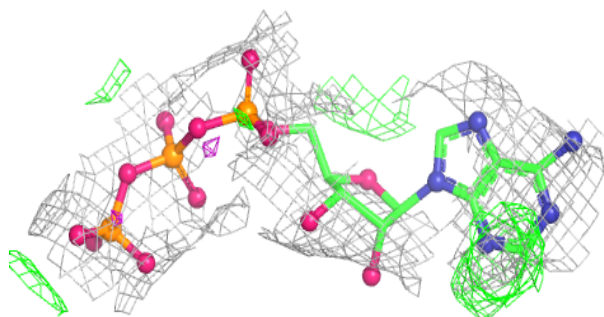
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	ATP	R	2101[A]	31/31	0.55	0.19	102,135,161,164	31
14	ATP	R	2101[B]	31/31	0.55	0.19	115,142,158,159	31
16	MG	A	1803	1/1	0.82	0.23	96,96,96,96	0
15	ZN	A	1801	1/1	0.93	0.06	214,214,214,214	0
15	ZN	L	101	1/1	0.96	0.06	182,182,182,182	0
15	ZN	A	1802	1/1	0.96	0.06	137,137,137,137	0
15	ZN	I	202	1/1	0.97	0.06	97,97,97,97	0
15	ZN	J	101	1/1	0.97	0.05	69,69,69,69	0
15	ZN	B	1301	1/1	0.98	0.04	157,157,157,157	0
15	ZN	I	201	1/1	0.98	0.05	114,114,114,114	0
15	ZN	C	401	1/1	0.99	0.06	105,105,105,105	0

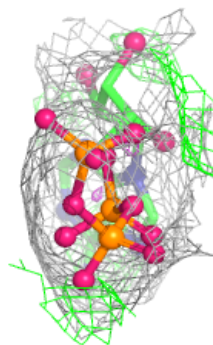
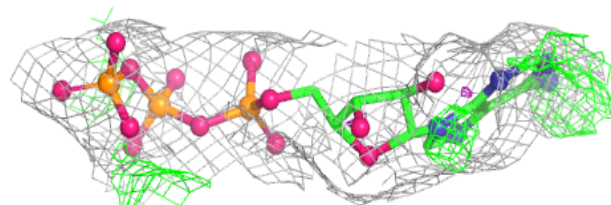
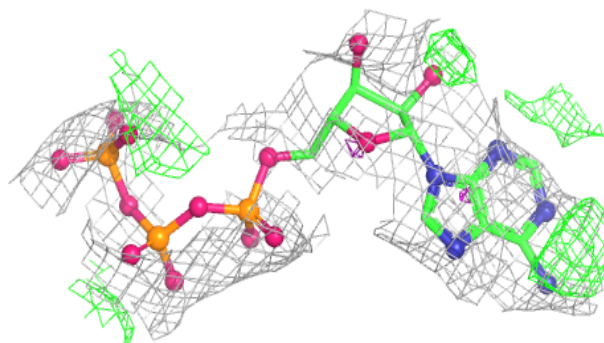
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP R 2101 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ATP R 2101 (B):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.